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Interaction between cationic and anionic surfactant using ultrasonic, physical and adiabatic parameters

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Surfactants are organic amphiphilic molecules having hydrophilic and hydrophobic parts in the same molecule. The relative densities, relative viscosities, specific conductance and ultrasonic velocity of sound of binary solutions of SDS-CTAB in water, formed in different mole fraction ratios, have been measured at 298 K and 308 K. From these data, the physical parameters such as adiabatic compressibility (β_{ad}), intermolecular free length (L_f), acoustic impedance (Z), relaxation time (τ) and molar free volume (V_f) have been evaluated using standard relations. The results are thus interpreted in terms of molecular interactions between cationic and anionic surfactants. Investigated value of physical properties thus defines that the molecular interaction is feasible and associative in nature and the determined acoustical and adiabatic parameters supports that nature.

Keywords: Ultrasonication, Ionic surfactants, Acoustic impedance, Molecular interaction

Surfactants are specific organic molecules having a hydrophobic alkyl chain tail part with affinity for the nonpolar phase and a hydrophilic head part with affinity for the polar phase in a single molecule[1-7]. Having this unique feature of holding two different parts in one molecule it shows amphiphilic nature. This amphiphilic nature made surfactant molecules of great importance. Surfactants have been of tremendous scientific importance because of their promising applications in many products like detergents, cosmetics, material fabrication, and drug delivery, among other areas. Sodium dodecyl Sulphate (SDS) is the most commonly used detergent in dentifrices[8]. They are classified as surface-active agents that lower the surface tension of water by absorbing at the liquid-gas interface[9], allowing easier spreading, and lowering the interfacial tension between two liquids. A surfactant can be classified by the presence of formally charged groups in its head, a nonionic surfactant has no charged group on its head part and an ionic surfactant carries a net charge on it[10]. If the charge is negative, the surfactant is called anionic; if the charge is positive, it is called cationic. Ionic surfactants are of great importance because of their major application in industries due to their useful properties in aqueous medium[11,12]. Ionic surfactants like anionic and cationic surfactants are useful in many non-similar fields like laundry[13-15], lipids recovery enhancers[16-19], pharmaceutical advantages[20-22], *etc*. The figures of both surfactants are shown in Fig. 1.

The present investigation aims at understanding the molecular interactions based on acoustical parameters and their excess functions in a mixed surfactant solution of anionic and cationic surfactant in water at 298K and 308K. We, therefore, investigated the different physical properties of the mixed surfactant solution at 298K and 308K. To obtain a piece of in-depth knowledge about the interactions between cationic and anionic surfactant, we prepared a wide range of solutions having different molar ratios of cationic and anionic surfactants in an aqueous medium. The physical properties and parameters of the individual surfactant SDS have been studied. Being one anionic and the other cationic surfactant,

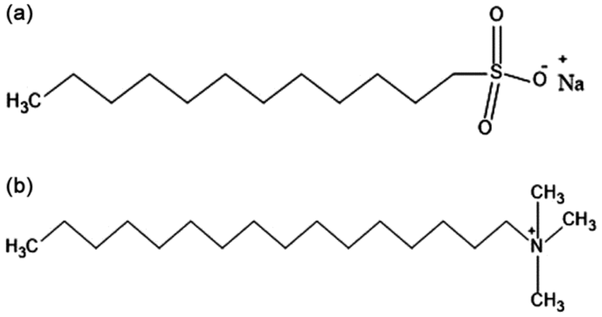

Fig. 1 — (a) Structure of SDS, (b) Structure of CTAB

they formed a precipitate on mixing. For better studies and explanation, we prepared different binary solutions of SDS and CTAB in varying values of their mole fractions. Physical and acoustical properties were thus investigated after mixing of SDS and CTAB solutions.

Experimental Section

Materials

Sodium dodecyl sulphate (SDS) supplied by Fisher Scientific of LR grade (purity >98%), and Cetyl trimethyl ammonium bromide (CTAB) brought from S.D. Fine Chemicals Ltd. (LR grade; purity>98%) had been used. For better results, both surfactants were purified with the help of recrystallization with ethanol. The glassware used was properly washed in aqua regia (1:3 HNO_3, HCl), sanitized, and autoclaved.

Methods

Ordinary chlorinated tap water of conductivity (2-5) x10^{-6} S·cm^{-1} at 298K was distilled with the help of a Millipore distillation unit. This water has further been distilled in the presence of alkaline potassium permanganate through a long vertical fractionating column of about 750 mm. The water thus obtained had conductivities of ≈ (1–4) × 10^{-7} S·cm^{-1} at 298K. Water thus purified was used throughout the whole experimental procedure.

Determination of Thermophysical parameters

Our study extended beyond traditional methods, incorporating diverse physical parameter analyses across different temperatures. Through this comprehensive approach, we aimed to unravel the complex molecular dynamics governing these interactions. These parameters are Relative density (ρ_r), Relative viscosity (V_r) and Ultrasonic velocity of sound (u) evaluated using equations (1) – (3).

Relative Density (ρ_r) measurements were done by the magnetic float densimeter kept in a constant heat reservoir using an equation (1):

$$\text{Relative Density } (\rho_r) = \frac{(W+w+f.I)}{(V+\frac{w}{d_{pt}})} \qquad \ldots(1)$$

Here, weight (w) is utilized, the current (I) passed through the circuit, the relative density of platinum (d_{pt}), the weight of platinum (W), and the volume of the float (V).

The relative viscosity (V_r) of diverse solutions was determined utilizing an electro-viscometer. Remarkably, the precision achieved in these measurements was approximately ±0.02%. It is evaluated using equation (2):

$$\frac{V_r}{V_w} = \frac{\rho_s}{\rho_w} . \frac{t_s}{t_w} \qquad \ldots(2)$$

The equation involves terms representing viscosity (V_w), density (ρ_w), and flow time (t_w) of water, alongside viscosity (V_r), density (ρ_s), and flow time (t_s) of the unknown liquid mixture.

The ultrasonic velocity of sound **(u)** was determined using a high-precision multi-frequency ultrasonic interferometer. This instrument, connected to a constant temperature water bath supplied by Mittal Enterprises, New Delhi, India, offers exceptional accuracy, with deviations of about ±0.1%. It was determined using the equation (3):

$$\text{Ultrasonic Velocity (u)} = \lambda . f \qquad \ldots(3)$$

Here, λ is the path difference and f applied frequency.

Determination of Acoustic Parameters

Elucidation of various Acoustic parameters had been done, leveraging insights from physical properties analyses. These parameters serve as invaluable indicators, offering nuanced insights into the behavior of molecular interactions within these systems. These parameters were determined using the physical parameters given using equations (4) – (8).

Adiabatic Compressibility **(β_{ad})** was elucidated using the equation (4):

$$\beta_{ad} = \frac{1}{\rho_r . u^2} \qquad \ldots(4)$$

Its unit is pascal^{-1}. Here $\boldsymbol{\rho_r}$ is the Relative Density and **u** is the ultrasonic velocity of the respective solution.

The Acoustic Impedance **(Z)** was elucidated using the equation (5):

$$z = \rho_r . u \qquad \ldots(5)$$

Its unit is Rayl. Here $\boldsymbol{\rho_r}$ is the relative density and **u** is the ultrasonic velocity of the respective solution.

The Intermolecular Free Length **(L_f)** was elucidated using the equation (6):

$$L_f = K_T . \beta_{ad}^2 \qquad \ldots(6)$$

Its unit is meters.

Here, $\mathbf{K_T}$ is the free length constant, which had been calculated using a formula,

$\mathbf{K_T}$ = (93.875 + 0.345T) x 10^{-8} , here, T is the temperature at which the experiment was performed.

At 298K, it valued 196.685 * 10^{-8} K and at 308K, it valued 200.135 * 10^{-8} K.

The viscous relaxation time **(τ)** was elucidated using the equation (7):

$$\tau = \frac{(4\,\mathrm{Vr}\,\beta_{\mathrm{ad}})}{3} \qquad \ldots(7)$$

Its unit is seconds. Here, $\mathbf{V_r}$ is Relative Viscosity & $\boldsymbol{\beta_{ad}}$ is Adiabatic Compressibility.

The Free Volume (V_f) associated can be calculated by using the equation,

$$V_f = [M_{eff}.\ \mu / K\ \eta]^{3/2} \qquad \ldots(8)$$

Here, M_{eff} is the effective mass, calculated as $M_{eff} = \Sigma\ M_i.\ X_i$

Where M is the molar mass and X is the mole fraction of the compound in the solution.

Results and Discussion

Thermophysical parameters analysis

The values of different thermophysical parameters were determined using equation **(1) – (3)**. The values of thermophysical parameters are shown in Table 1 and Table 2.

The table shows all the experimental values of the determined physical properties of different solutions. The value of Density, Viscosity, and Ultrasonic velocity of sound increases as the mole fraction of CTAB increases through a unique mixed surfactant solution. This increase in densities, viscosities and ultrasonic velocity of sound values and decrease in Specific Conductance values is may be due to cohesive forces, thus supporting the concept of molecular association means there is type of attraction force happening between the molecules[25,26].

Viscosity is the most important property of liquid to study. In fluid dynamics, it is a useful parameter that governs the thickness or thinness of a given fluid. Viscosity describes a liquid's resistance to flow under an applied pressure from one layer of liquid to the next layer. As viscosity increases, the resistance between two-layer increases. The increase in viscosity might be due to the increase of molecular attraction forces acting between the molecules in the solution.

Ultrasonic sound travels through various materials under the influence of sound pressure. In the liquid state of matter, the atoms or molecules are bounded or attracted by one another through some interactive molecular interactions that cause excess pressure resulting in sound wave propagation through the experimental liquid[27]. The studies on frequency of the ulcers determined earlier describes about the adverse effect of SDS as it is a significantly higher frequency of aphthous ulcers was demonstrated when the patients brushed with an SLS- than with a CAPB-

Table 1 — Physical parameters determined at 298K

Mole fraction ratio of SDS:CTAB	Specific Conductance (K) mS cm^{-1}	Relative Density (ρ) Kg/m^3	Ultrasonic Velocity (U) m/s	Relative Viscosity mPa sec^{-1}
01 : 00	0.166	998.27	1508.460	0.9538
0.9 : 0.1	0.15	1006.06	1510.746	0.9581
0.88 : 0.12	0.146	1006.94	1512.125	0.9613
0.86 : 0.14	0.143	1007.67	1513.891	0.9652
0.84 : 0.16	0.139	1008.03	1515.273	0.9694
0.82 : 0.18	0.137	1008.98	1517.634	0.9796
0.80 : 0.20	0.135	1009.72	1518.571	0.9849
0.78 : 0.22	0.132	1011.15	1521.440	0.9918
0.76 : 0.24	0.128	1012.41	1524.780	1.1002

Table 2 — Physical parameters determined at 298K and physical parameters determined at 308K

Mole fraction ratio of SDS:CTAB	Specific Conductance (K) mS cm^{-1}	Relative Density (ρ) Kg/m^3	Ultrasonic Velocity (U) m/s	Relative Viscosity mPa sec^{-1}
01: 00	0.204	998.04	1504.71	0.9479
0.9 : 0.1	0.191	1003.89	1507.143	0.9506
0.88 : 0.12	0.188	1004.24	1508.785	0.9573
0.86 : 0.14	0.185	1004.98	1510.008	0.9619
0.84 : 0.16	0.183	1005.62	1511.171	0.9684
0.82 : 0.18	0.179	1006.71	1512.981	0.9717
0.80 : 0.20	0.176	1008.18	1514.863	0.9793
0.78 : 0.22	0.173	1009.51	1516.157	0.9856
0.76 : 0.24	0.169	1010.16	1518.62	1.0872

containing or a detergent-free placebo paste. An SLS-free toothpaste may thus be recommended for patients with recurrent aphthous ulcers[28].

Acoustic Parameters Analysis

The acoustic parameters determined using equation (4) – (8) were shown in Table 3, Table 4, Table 5, Table 6 and Table 7. The variation of trends is better understood using the bar diagrams which are shown in Fig. 2, Fig. 3, Fig. 4, Fig. 5 and Fig. 6.

The function of thermodynamic adiabatic compressibility is the fractional decrease of volume per unit increase of absolute pressure when no heat change is involved in the process. As from Table 3, there is a decrease in the value of adiabatic compressibility as the mole fraction of CTAB increases. This is due to the influence of surrounding differently charged Surfactant molecules and water molecules, which leads to an increase in pressure and thus the solution becomes harder to compress. This decrease in adiabatic compressibility with an increase in mole fraction of CTAB shows strong solute-solvent interaction.

Intermolecular Free Length L_f is the distance covered by the sound wave between the neighbouring molecule surfaces. It is a measure of intermolecular interactions between the components in binary solutions. The increase or decrease in free length indicates the weakening and strengthening of intermolecular interaction. From Table 4, it is seen that as the ultrasonic velocity increases due to an increase in either density or concentration, the intermolecular free length has to increase and vice-versa. From Table 4, the intermolecular free length decreases with an increase in the mole fraction of CTAB in a mixed surfactant solution. This decrease in free length indicates that there is a significant attraction between the SDS and CTAB in the mixed surfactant solution.

As the value of the mole fraction of CTAB increases, value of Acoustical impedance, shown in

Table 3 — Variation of Adiabatic Compressibility

Mole fraction ratio of SDS : CTAB	Adiabatic Compressibility $\beta_{ad}\times10^{-12}$ (pascal)$^{-1}$	
	298K	308K
01 : 00	4.35505	4.38533
0.9 : 0.1	4.34221	4.37429
0.88 : 0.12	4.33004	4.36296
0.86 : 0.14	4.3206	4.35351
0.84 : 0.16	4.30312	4.33837
0.82 : 0.18	4.29366	4.32128
0.80 : 0.20	4.26143	4.30623
0.78 : 0.22	4.18971	4.29151
0.76 : 0.24	4.19794	4.22543

Table 4 — Variation of Intermolecular Free Length

Mole Fraction ratio of SDS : CTAB	Intermolecular Free Length $L_f\times10^{-10}$ meter	
	298K	308K
1:00	4.1794	4.1962
0.9 : 0.1	4.1540	4.1858
0.88 : 0.12	4.1494	4.1803
0.86 : 0.14	4.1398	4.1774
0.84 : 0.16	4.1311	4.1685
0.82 : 0.18	4.1254	4.1603
0.8 : 0.2	4.1203	4.1531
0.78 : 0.22	4.1089	4.1460
0.76 : 0.24	4.0836	4.1210

Table 5 — Variation of Acoustic Impedanceb

mole fraction ratio of SDS : CTAB	Acoustic Impedance $\times10^{4}$ (rayl)	
	298K	308K
1:00	150.735	150.176
0.9 : 0.1	151.991	151.301
0.88 : 0.12	152.262	151.519
0.86 : 0.14	152.550	151.753
0.84 : 0.16	152.744	152.314
0.82 : 0.18	153.126	152.717
0.8 : 0.2	153.433	153.058
0.78 : 0.22	154.071	153.605
0.76 : 0.24	154.569	153.918

Table 6 — Variation of Relaxation time

mole fraction ratio of SDS : CTAB	Relaxation time $\times10^{-8}$ sec	
	298K	308K
1:00	62.316	61.644
0.9 : 0.1	60.872	59.289
0.88 : 0.12	58.937	58.227
0.86 : 0.14	58.104	57.873
0.84 : 0.16	57.831	56.136
0.82 : 0.18	56.729	55.072
0.8 : 0.2	56.347	54.194
0.78 : 0.22	56.072	53.684
0.76 : 0.24	55.616	53.279

Table 7 — Variation of Free Volume

Mole fraction ratio of SDS : CTAB	Free Volume $V_f\times10^{-7}$ m^3 mol^{-1}	
	298K	308K
1:00	7.0971	7.8732
0.9 : 0.1	7.0236	7.8161
0.88 : 0.12	7.0014	7.6274
0.86 : 0.14	6.9641	7.4916
0.84 : 0.16	6.7917	7.2463
0.82 : 0.18	6.6166	7.1074
0.8 : 0.2	6.5074	6.9891
0.78 : 0.22	6.3901	6.6827
0.76 : 0.24	6.2874	6.5691

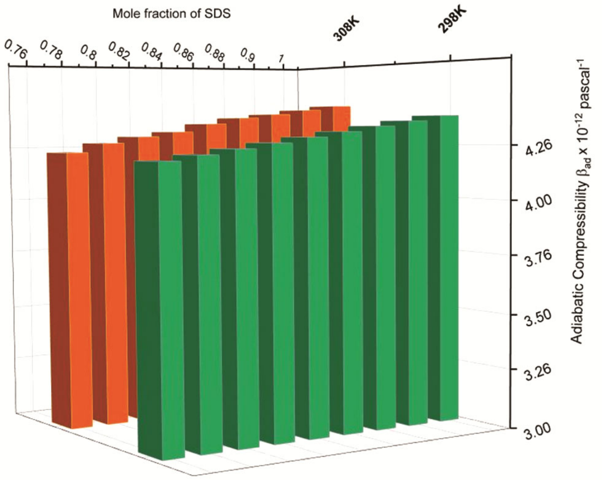

Fig. 2 — Bar diagram showing variation of adiabatic compressibility

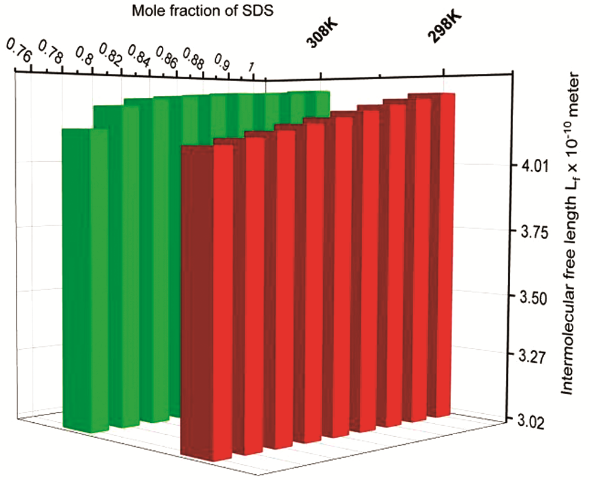

Fig. 3 — Bar diagram showing variation of Intermolecular free length

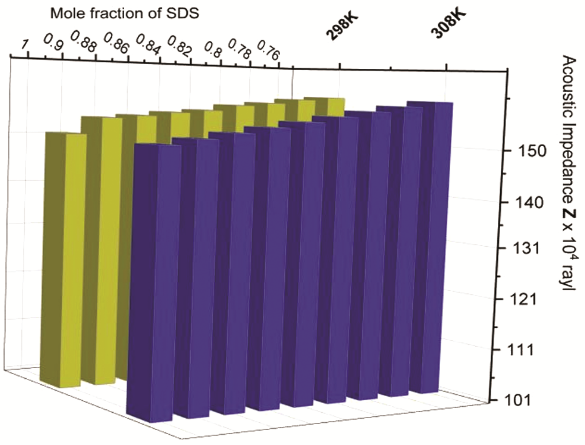

Fig. 4 — Bar diagram showing variation of acoustic impedance

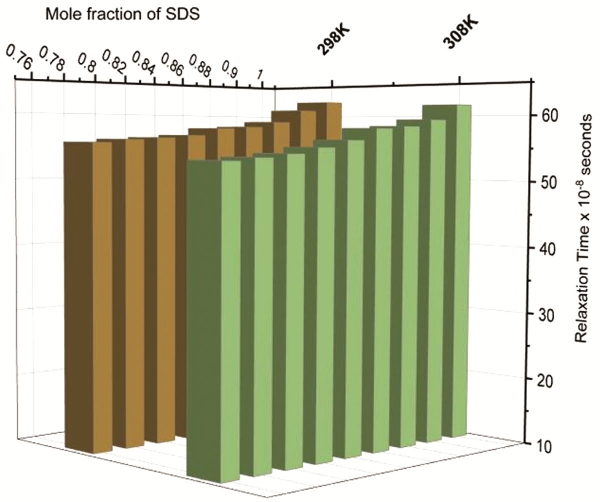

Fig. 5 — Bar diagram showing variation of relaxation time

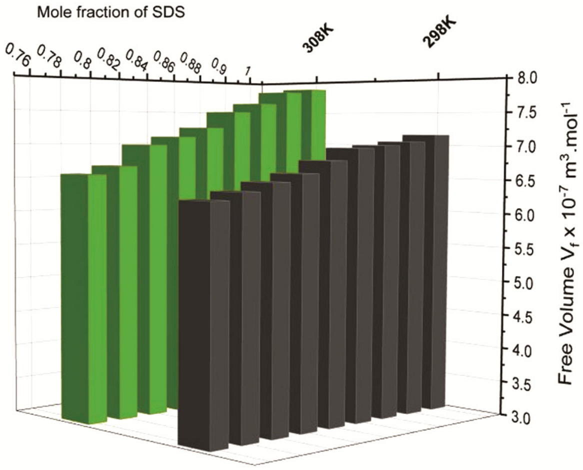

Fig. 6 — Bar diagram showing variation of free volume

Table 5, which is the ratio of complexity between effective pressure exerted by sound and particle velocity, increases. This increase in acoustical impedance confirms that the molecular interactions are associative in nature, and the force of attraction increases between SDS and CTAB as the mole fraction of CTAB increases in different ratio solutions.

Relaxation time is the time taken for the excitation energy to appear as translational energy, it depends upon the temperature and impurities[29]. The dispersion of the ultrasonic velocity in SDS/CTAB binary solution in water reveals information about the characteristic time of the relaxation process that causes dispersion. Table 6 shows the value of relaxation time decreases as the resting time between the molecules decreases with an increase in the amount of added CTAB in oppositely charged SDS solution which supports that the molecular interactions are associative in nature.

Free volume, shown in Table 7, is one of the significant factors in explaining the variations in the physicochemical properties of liquids and liquid mixtures. The free volume and its dependent properties have a close connection with molecular structure, showing an interesting feature about the interactions that may occur when oppositely charged SDS and CTAB mixed solution formation takes place[30].

The molecular interaction between like and unlike molecules is influenced by structural arrangements along with the shape and size of the molecules. Eyring and Kincaid defined free volume as the effective volume in which a particular atom or molecule of the liquid solution can move and obey perfect gas laws. Free volume is an indirect measure of the volume that is vacant between the solute-solvent molecules. The effective volume is a volume in which the molecules show random motion due to the effect of the repulsion from neighbouring molecules. The decreasing trend of the free volume shows the occupation of an attractive force between solute and solvent molecules as well as in between two solute molecules and also signifies the possibility of ion-solvent interaction.

Conclusion

The density, viscosity, and ultrasonic velocity measurements show that all the properties are increasing and specific conductance decreases as the added amount of CTAB in SDS solution increases at 298K & 308K. The variation of physical parameters with increasing mole fraction of CTAB in SDS solution shows that the molecular attraction between the SDS and CTAB in aqueous solution is associative in nature. That means there is an attraction force between negatively charged SDS molecules and positively charged CTAB molecules. All investigated physical properties as well as evaluated parameters support this result with their variation in the mole fraction of added cationic surfactant's CTAB in anionic surfactant's SDS solution. The decrease in value of the specific conductivity ensures that the number of free ions responsible for conductivity decreases with increase in mole fraction of CTAB through different SDS solutions.

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Conflict of Interests

There are no competing interests declared by all authors.

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Author's contributions statement

Aditya Gupta completed all the Experimental work and calculations. Divyanshi Mishra was involved in the manuscript preparation, data collection and interpretation. Under Indu Saxena's supervision, this article granted final permission to the published version.

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